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Electric Field-Driven Water Dipoles: Nanoscale Architecture of Electroporation
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Electroporation, the permeabilization of cell membranes by applied electric fields, is widely used in biology, biotechnology and medicine. However, the lack of understanding of the molecular mechanism of electroporation has seriously limited our ability to develop predictive, quantitative models that would enable efficient optimization and improvement of electroporation protocols. We propose a new molecular mechanism for the electroporation of a lipid bilayer based on a structural and energetics analysis of trajectories produced by molecular dynamics simulations. We demonstrate that electropore formation is driven by the reorganization of interfacial water molecules as they increasingly align with an external electric field. Although the contributing role of water in electroporation has been noted previously, here we propose that interfacial water is the main player in the process, its initiator and driver. The role of membrane lipids, to a first-order approximation, is that of a relatively passive barrier to pore formation. This new view significantly simplifies the study of electroporation and opens up new opportunities for both theoretical and experimental research for improvements in existing methods or to use this phenomenon in new, innovative ways.

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Non-Equilibrium Computation of Diffusion Constants for Water, Lipids and Proteins
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We investigated the self-diffusivity of water, solvated DPPC and other systems in near-equilibrium conditions by applying a constant force on selected molecules. The mobility constant and diffusion coefficient was calculated from the obtained terminal drift velocity. To reduce the background noise from the thermal fluctuations, we ran multiple simulations of different initial conditions and averaged the data over the ensemble. The results are generally found to be within a factor of 1.5 of the experimental constants. Compared to the traditional method of using mean-square displacement, this technique offers both a much faster convergence rate and a well-suited scheme for parallelization.

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Characterization of Pure Lipid Bilayers using Molecular Dynamics Simulations
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Understanding individual lipid interactions and properties will provide information that can be used to better understand the role of specific lipid types to the properties of a real cell membrane. After determining a lipid's structure, specifically the head and the tail type, it is then critical to understand how it behaves and interacts when packed in a lipid bilayer membrane. This research project aims to use molecular dynamics simulations to study basic lipid properties, such as the area per lipid and bilayer thickness, when a specific lipid is packed in a homogenous bilayer membrane. We have made and simulated a total of 115 homogenous bilayer systems using all the lipid types available in CHARMM-GUI Membrane Builder. The simulation results will be presented in terms of the effects of head, tail, and temperature on the basic lipid properties. In particular, the resulting per-lipid area of each lipid will be used as the initial lipid area for this lipid in the CHARMM-GUI Membrane Builder.

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Measurements of Solute Polarizabilites Affecting Lipid Membrane Interactions
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The van der Waals attraction between lipid membranes depends on the polarizability of solute molecules present in the aqueous space between neighboring membranes [1]. In particular, zwitterionic molecules (such as common pH buffers) have been shown to affect van der Waals forces more strongly than monovalent saltions [2]. Experimentally, changes in van der Waals forces are detected by x-ray scattering measurements of multilamellar lipid vesicles through the sensitivity of lamellar repeat distances to solution polarizabilities. In this respect, a direct determination of solute polarizabilities would lend support to the interpretation of x-ray data. Here we use a recently developed method [3] to quantify the polarizabilities of zwitterionic pH buffers including TAPS, TES, MES, MOPS, and HEPES. This method calculates a solution function $r(c)$ which gives the polarizability of hydrated solutes as a function of concentration (c) by combining mass density and index of refraction measurements into a dimensionless quantity. We obtain that the zwitterionic molecules considered are significantly more polarizable than NaCl used as reference. These results are in agreement with x-ray measurements of lipid membrane interactions in the presence of buffers and monovalent salt solutions. Further, measurements of solutions 1:1 mixtures by volume have shown the polarizability is additive in agreement with theoretical models.

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Effect of Lipid Recycling on the Finite Size of Lipid Rafts in Symmetric and Asymmetric Bilayers
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The plasma membrane of eukaryotic cells is composed of various types of lipids and is thought to form lipid rafts, which are nanoscale domains, as a result of phase separation. It is well documented that giant unilamellar vesicles, composed of a saturated lipid, an unsaturated lipid and cholesterol, exhibit phase separation with large micron-scale domains, limited in size only by the finite size of the vesicle itself. In contrast, lipid domains in the plasma membrane are orders of magnitude smaller. The cause of the finite nanoscale size of these lipid rafts in biological systems remains poorly understood. The present research uses molecular dynamics of an implicit-solvent molecular model of self-assembled multi-component lipid membranes to investigate lipid recycling due to trafficking. In particular, the goal of this research is to investigate whether trafficking affects the size of lipid rafts. Our systematic simulations for varying recycling rate as well as the transbilayer lipid distribution and lipid composition in each leaflet show that the system achieves a non-equilibrium steady state with a microphase separation. The length scale of the micro-phase separated domains is found to decrease with increasing the rate of recycling. An extrapolation of our data to recycling rates comparable to biological values lead to an average domain size approaching the size of lipid rafts in plasma membranes.

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Surface Properties and Membrane Packing in Hybrid Liposomes Composed of Tetraether and Diester Lipids
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Archaeal bipolar tetraether lipids are extraordinarily stable against biochemical and physical stressors and non-toxic to animals; thus, they are appealing biomaterials that hold great promise for technological applications. Here, we used electrophoretic mobility measurements and TNS fluorescence to determine zeta potential and surface potential of liposomes (~150 nm in diameter) composed of archaeal tetraether lipids and conventional diester lipids. We also used Laurdan fluorescence to explore membrane packing in the same membrane system. The polar lipid fraction E (PLFE) from the archaeon *S. acidocaldarius* was used as the tetraether component. PLFE lipids are asymmetric macrocyclic molecules carrying a negative charge on the phosphate moiety at one of the two polar ends at neutral pH. We found that zeta potential varies with PLFE content in a biphasic manner, being most negative when the PLFE content is ~60 mol%. Surface potential is also PLFE content dependent, showing a minimum at ~50 mol% PLFE. On the other hand, Laurdan GP (generalized polarization) data, inferentially membrane packing, displays a peculiar behavior at 20-40 mol% PLFE. In a separate study, we used the AAPH-induced Laurdan fluorescence intensity change to deduce information about membrane packing. AAPH (2,2'-azobis (2-amidinopropane) dihydrochloride) is a water-soluble, free-radical generator. Upon addition of AAPH, there was a lag time (t), followed by a steady decrease in Laurdan fluorescence intensity due to probe oxidation. The t values as well as the initial rate (R) of AAPH-induced Laurdan oxidation were found to change with PLFE mole fraction in a non-monotonic manner, showing an anomaly between 20-50 mol % PLFE. These data together suggest that, in the range 20-50 mol %, these hybrid liposomes undergo major structural changes engendered by PLFE content.

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Effects of Dehydration-Rehydration on the Structural and Functional Properties of Pulmonary Surfactant
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Pulmonary surfactant is a lipoproteic complex, which main function is to stabilize the respiratory air-liquid interface. Lack or inactivation of surfactant is